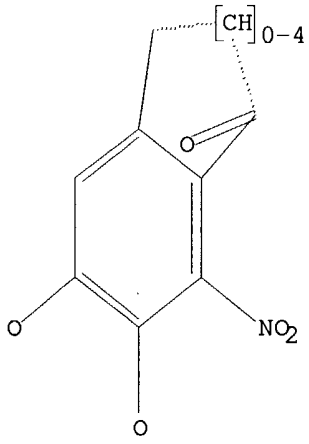

Structure attributes must be viewed using STN Express query preparation.

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=> d l2
L2 HAS NO ANSWERS
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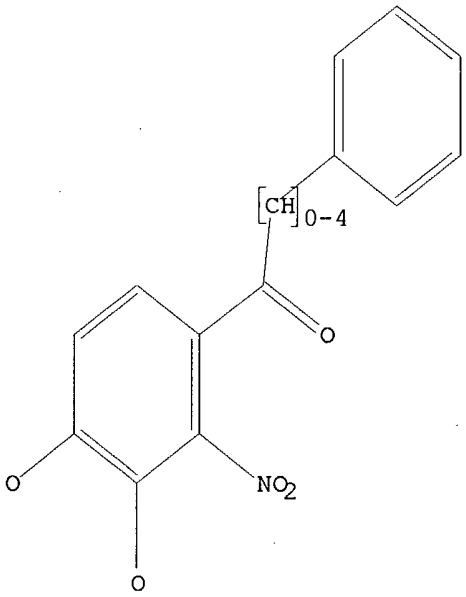

Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 17:44:53 FILE 'REGISTRY'

aq/885,855

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FULL SCREEN SEARCH COMPLETED -    178 TO ITERATE

100.0% PROCESSED     178 ITERATIONS                          10 ANSWERS
SEARCH TIME: 00.00.01

L3           10 SEA SSS FUL L1

=> s l2 sss full
FULL SEARCH INITIATED 17:44:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     63 TO ITERATE

100.0% PROCESSED      63 ITERATIONS                          29 ANSWERS
SEARCH TIME: 00.00.01

L4           29 SEA SSS FUL L2

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               311.68     311.89

FILE 'CAPLUS' ENTERED AT 17:45:05 ON 10 SEP 2004
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FILE COVERS 1907 - 10 Sep 2004  VOL 141 ISS 12
FILE LAST UPDATED: 9 Sep 2004  (20040909/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l3
L5           2 L3

=> s l4
L6           5 L4

=> s l3 or l4
             2 L3
             5 L4
L7           6 L3 OR L4

=> d l5 1-2 ibib abs hitstr

L5   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2001:935557  CAPLUS
DOCUMENT NUMBER:          136:69653
```

09/885,855

TITLE: Preparation of substituted nitrated catechols as catechol O-methyl transferase inhibitors for the treatment of central and peripheral nervous system disorders

INVENTOR(S): Learmonth, David Alexander; Soares da Silva, Patricio Manuel Vieira

PATENT ASSIGNEE(S): Portela & CA SA, Port.

SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2

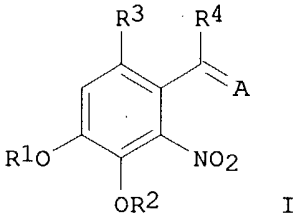
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098250	A1	20011227	WO 2001-GB2774	20010621
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002037931	A1	20020328	US 2001-885855	20010620
EP 1167341	A1	20020102	EP 2001-305373	20010621
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
GB 2365864	A1	20020227	GB 2001-15223	20010621
GB 2365864	B2	20021120		
BR 2001011897	A	20030513	BR 2001-11897	20010621
JP 2004501129	T2	20040115	JP 2002-504206	20010621

PRIORITY APPLN. INFO.: GB 2000-15228 A 20000621
WO 2001-GB2774 W 20010621

OTHER SOURCE(S): MARPAT 136:69653

GI



I

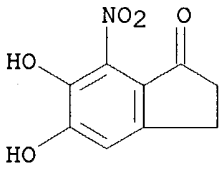
AB Title compds. I [wherein R1 and R2 = independently H or (un)substituted alkanoyl, aroyl, alkoxycarbonyl, or alkylcarbamoyl; R3 = H or (un)substituted alkanoyl or aroyl; R4 = (un)substituted alkyl or aryl; or R4 taken together with R3 = (un)substituted carbocycle; A = O, NR5, or (un)substituted alkylidene; R5 = NHR6 or OR7; R6 = (un)substituted alkyl or aryl; R7 = H, alkyl, or alkanoyl; with provisos] were prepared as catechol O-Me transferase (COMT) inhibitors. In COMT oral bioavailability, half-life, and brain access assays, some invention compds. demonstrated enhanced access to the brain and limited activity in

the periphery offering improved selectivity for mood disorder therapy. Others demonstrated limited access to the brain and enhanced activity in the periphery offering improved selectivity for treatment of Parkinson's disease and parkinsonian disorders, gastrointestinal disturbances, edema formation states and hypertension. Thus, bromination of 3,4-dihydroxy-2-nitroacetophenone with phenyltrimethylammonium tribromide in THF to give the α-bromoketone, followed by addition of morpholine in MeCN, afforded 1-(3,4-dihydroxy-2-nitrophenyl)-2-morpholin-4-ylethanone. The latter inhibited COMT activity in homogenates of rat liver and brain and SK-N-SH cells at 0.8 0.2%, 13 0%, and 27 0%, resp., compared to control.

IT **383382-47-6P**, 5,6-Dihydroxy-7-nitroindan-1-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; preparation of substituted nitrated catechols as COMT inhibitors for treatment of central and peripheral nervous system disorders)

RN 383382-47-6 CAPLUS

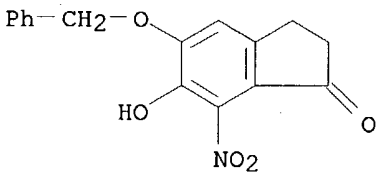
CN 1H-Inden-1-one, 2,3-dihydro-5,6-dihydroxy-7-nitro- (9CI) (CA INDEX NAME)



IT **383382-45-4P**, 5-Benzyloxy-6-hydroxy-7-nitroindan-1-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted nitrated catechols as COMT inhibitors for treatment of central and peripheral nervous system disorders)

RN 383382-45-4 CAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-6-hydroxy-7-nitro-5-(phenylmethoxy)- (9CI) (CA INDEX NAME)

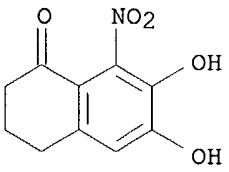


IT **383382-48-7P**, 6,7-Dihydroxy-8-nitro-3,4-dihydro-2H-naphthalen-1-one **383382-62-5P**, 5,6-Dihydroxy-2-morpholin-4-ylmethyl-7-nitroindan-1-one **383382-63-6P**, 5,6-Dihydroxy-7-nitro-2-piperidin-1-ylmethylindan-1-one **383382-64-7P**, 5,6-Dihydroxy-7-nitro-2-[4-(3-trifluoromethylphenyl)piperazin-1-ylmethyl]indan-1-one **383382-65-8P**, 5,6-Dihydroxy-7-nitro-2-(4-phenylpiperazin-1-ylmethyl)indan-1-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted nitrated catechols as COMT inhibitors for

treatment of central and peripheral nervous system disorders)

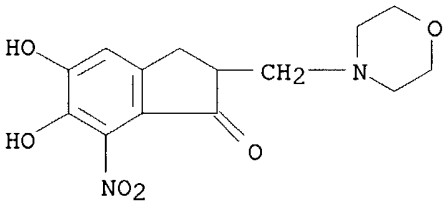
RN 383382-48-7 CAPLUS

CN 1(2H)-Naphthalenone, 3,4-dihydro-6,7-dihydroxy-8-nitro- (9CI) (CA INDEX NAME)



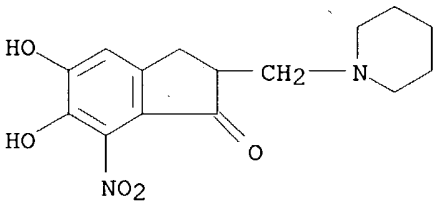
RN 383382-62-5 CAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5,6-dihydroxy-2-(4-morpholinylmethyl)-7-nitro- (9CI) (CA INDEX NAME)



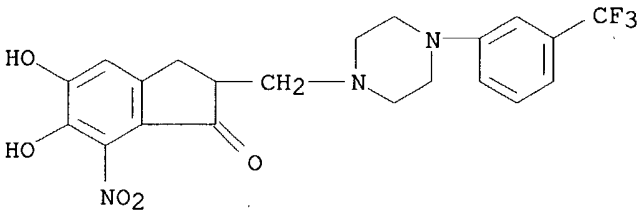
RN 383382-63-6 CAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5,6-dihydroxy-7-nitro-2-(1-piperidinylmethyl)- (9CI) (CA INDEX NAME)



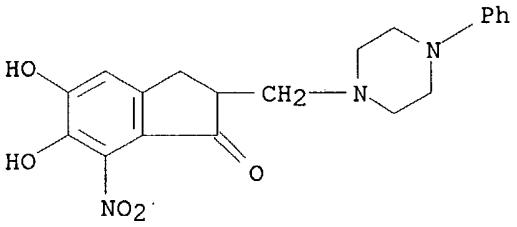
RN 383382-64-7 CAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5,6-dihydroxy-7-nitro-2-[[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)

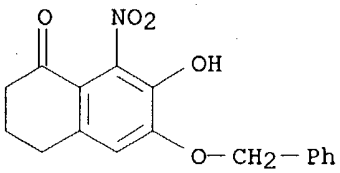


RN 383382-65-8 CAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5,6-dihydroxy-7-nitro-2-[(4-phenyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)



IT **383383-11-7**, 6-Benzyloxy-7-hydroxy-8-nitro-3,4-dihydro-2H-naphthalen-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of substituted nitrated catechols as COMT inhibitors for treatment of central and peripheral nervous system disorders)
RN 383383-11-7 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-7-hydroxy-8-nitro-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

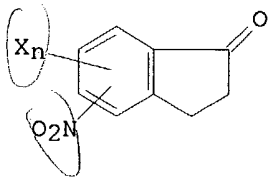


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:501857 CAPLUS
DOCUMENT NUMBER: 89:101857
TITLE: Nitro-1-indanones fungicides
INVENTOR(S): Takahi, Yukiyoshi; Yura, Yasuo
PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53012421	A2	19780203	JP 1976-86248	19760720
PRIORITY APPLN. INFO.:			JP 1976-86248	19760720

GI



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JP 53012421 A 2

JP 53012421

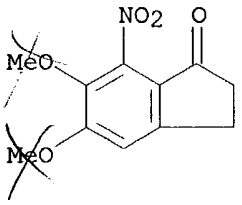
09/885,855

AB The title compds. I (X = lower alkyl, lower alkoxy, halogen, or OH; n = 1-3) prepared either by nitration of the appropriate indanone or by ring closure of a substituted phenylpropionic acid are fungicides. Thus, 300 ppm 4-nitro-5-methyl-1-indanone [66773-14-6] prevented Piricularia infection in rice.

IT **66773-29-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and fungicidal activity of)

RN 66773-29-3 CAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5,6-dimethoxy-7-nitro- (9CI) (CA INDEX NAME)



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L6 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:77702 CAPLUS
DOCUMENT NUMBER: 138:137024
TITLE: Regioselective nitration of phenolic compounds into ortho-nitrophenolic compounds using alkyl nitrates as the nitration agents
INVENTOR(S): Learmonth, David Alexander
PATENT ASSIGNEE(S): Portela & C.A., S.A., Port.
SOURCE: Brit. UK Pat. Appl., 21 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

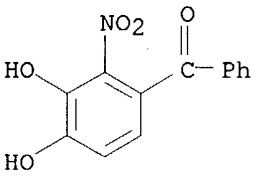
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2377934	A1	20030129	GB 2001-18139	20010725
JP 2003055214	A2	20030226	JP 2001-303847	20010928
WO 2003011810	A1	20030213	WO 2002-GB3356	20020722
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1409446	A1	20040421	EP 2002-747586	20020722
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
PRIORITY APPLN. INFO.: GB 2001-18139 A 20010725
WO 2002-GB3356 W 20020722
OTHER SOURCE(S): CASREACT 138:137024; MARPAT 138:137024

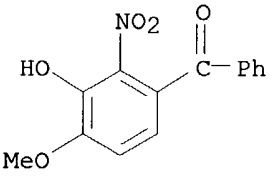
AB A method for the regioselective ortho-directed nitration of phenolic compds. (e.g., phenol) into 2-nitrophenols (e.g., 2-nitrophenol), useful as intermediates for the preparation of compds. useful against nervous system disorders (no data), is described which employs a (cyclo)alkyl nitrate (e.g., iso-Pr nitrate) as the nitration agent.

IT **383382-84-1P 491832-39-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regioselective nitration of phenolic compds. into ortho-nitrophenolic compds. using alkyl nitrates as the nitration agents)

RN 383382-84-1 CAPLUS
CN Methanone, (3,4-dihydroxy-2-nitrophenyl)phenyl- (9CI) (CA INDEX NAME)

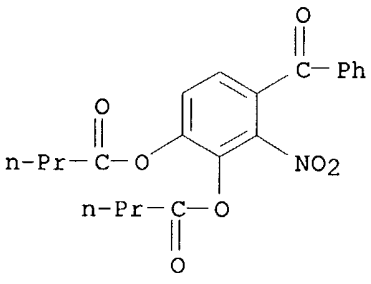


RN 491832-39-4 CAPLUS
CN Methanone, (3-hydroxy-4-methoxy-2-nitrophenyl)phenyl- (9CI) (CA INDEX NAME)

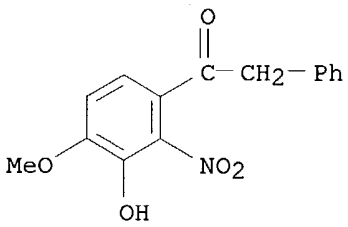


IT **383382-83-0P 491832-40-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective nitration of phenolic compds. into ortho-nitrophenolic compds. using alkyl nitrates as the nitration agents)

RN 383382-83-0 CAPLUS
CN Butanoic acid, 4-benzoyl-3-nitro-1,2-phenylene ester (9CI) (CA INDEX NAME)



RN 491832-40-7 CAPLUS
CN Ethanone, 1-(3-hydroxy-4-methoxy-2-nitrophenyl)-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:5916 CAPLUS
DOCUMENT NUMBER: 138:73466
TITLE: Preparation of nucleotide photolabile esters capable of generating acid on photolysis in solid phase synthesis of nucleic acids
INVENTOR(S): Serafinowski, Pawel Jerzy; Garland, Peter Bryan
PATENT ASSIGNEE(S): The Institute of Cancer Research, UK
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Sand assignee date not good West: no U.S. case

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000644	A1	20030103	WO 2002-GB2896	20020621
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1399412	A1	20040324	EP 2002-740905	20020621
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.:
GB 2001-15231 A 20010621
GB 2001-22760 A 20010921
WO 2002-GB2896 W 20020621

OTHER SOURCE(S): MARPAT 138:73466
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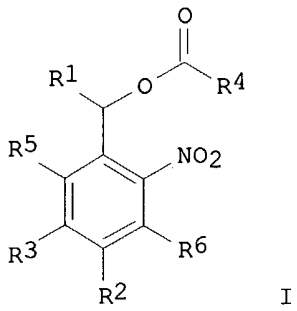


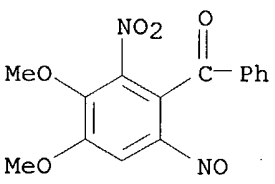
I

AB Nucleotides I wherein: R1 is selected from hydrogen, aryl or substituted aryl, aryloxy or substituted aryloxy, or an unsubstituted or substituted heterocyclic group; R2 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, or a nitro group; R3 is selected from hydrogen, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, or an unsubstituted or substituted heterocyclic group; R4 is an alkyl group substituted with one or more halogen substituents; R5 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, a nitro group or an unsubstituted or substituted heterocyclic group; and, R6 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, or amino or substituted amino, or an unsubstituted or substituted heterocyclic group, which are capable of generating acid on photolysis are disclosed, and the uses of these compds., especially for deprotecting the termini of nucleic acid mols. or peptides during synthesis of arrays. The compds. described herein may be employed in the detritylation of 5'-O-dimethoxytrityl (DMT) protected nucleotides by photolyzing the compds. to generate an acid capable of removing the DMT group allowing oligonucleotide arrays to be synthesized using readily available 5'-O-DMT-nucleoside-3'-O-phosphoramidite monomers conventionally used in solid phase nucleic acid synthesis. A method of avoiding the effects of stray light in projection lithog. techniques is also disclosed. Thus, α-phenyl-4,5-dimethoxy-2,6-dinitrobenzyltrichloroacetate was prepared and used in synthesis od DNA.

IT **479637-77-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nucleotide photolabile esters capable of generating acid on photolysis in solid phase synthesis of DNA)

RN 479637-77-9 CAPLUS

CN Methanone, (3,4-dimethoxy-2-nitro-6-nitrosophenyl)phenyl- (9CI) (CA INDEX NAME)



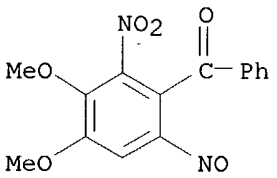
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:29 CAPLUS
DOCUMENT NUMBER: 138:188006
TITLE: Novel Photo-Acid Generators for Photo-Directed Oligonucleotide Synthesis
AUTHOR(S): Serafinowski, Pawel J.; Garland, Peter B.
CORPORATE SOURCE: Cancer Research UK Centre for Cancer Therapeutics and Section of Molecular Carcinogenesis, Institute of Cancer Research, Surrey, SM2 5NG, UK
SOURCE: Journal of the American Chemical Society (2003), 125(4), 962-965
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:188006

AB Photo-directed oligonucleotide synthesis uses either direct or indirect light-dependent 5'-deprotection. Both have been reported to give lower stepwise synthetic yields than conventional methods. The deficiency appears to be due to incomplete deprotection at the oligonucleotide 5'-position and, addnl. in the case where photo-direction is indirect and uses photo-generated photo-acid to effect 5'-detritylation, the depurinating effects of strong acid. We have developed novel photosensitive-2-nitrobenzyl esters that on irradiation with near UV light generate α-chloro-substituted acetic acids, such as trichloroacetic acid, which are widely and successfully used in conventional solid-phase oligonucleotide synthesis. α-Phenyl-4,5-dimethoxy-2-nitrobenzyltrichloroacetate and α-phenyl-4,5-dimethoxy-2,6-dinitrobenzyltrichloroacetate showed appropriate photochem. characteristics and were used for photo-directed synthesis of a variety of oligonucleotides, including (T)5, TATAT, TGTGT, (T)10, (AT)5, (CT)5 (GT)5, and (TGCAT)2 on a modified millipore expedite DNA synthesizer. The outcomes were compared with those obtained by use of directly added trichloroacetic acid (conventional synthesis). The stepwise yields for the two methods were essentially identical.

IT **479637-77-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(photo-acid generators for photo-directed oligonucleotide solid-phase synthesis and photochem. detritylation of DNA)
RN 479637-77-9 CAPLUS
CN Methanone, (3,4-dimethoxy-2-nitro-6-nitrosophenyl)phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:935557 CAPLUS
DOCUMENT NUMBER: 136:69653

09/885,855

TITLE: Preparation of substituted nitrated catechols as catechol O-methyl transferase inhibitors for the treatment of central and peripheral nervous system disorders

INVENTOR(S): Learmonth, David Alexander; Soares da Silva, Patricio Manuel Vieira

PATENT ASSIGNEE(S): Portela & CA SA, Port.

SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2

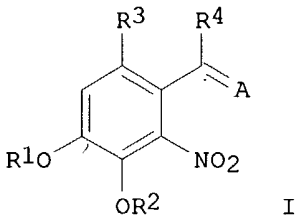
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098250	A1	20011227	WO 2001-GB2774	20010621
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002037931	A1	20020328	US 2001-885855	20010620
EP 1167341	A1	20020102	EP 2001-305373	20010621
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
GB 2365864	A1	20020227	GB 2001-15223	20010621
GB 2365864	B2	20021120		
BR 2001011897	A	20030513	BR 2001-11897	20010621
JP 2004501129	T2	20040115	JP 2002-504206	20010621

PRIORITY APPLN. INFO.: GB 2000-15228 A 20000621
WO 2001-GB2774 W 20010621

OTHER SOURCE(S): MARPAT 136:69653

GI



I

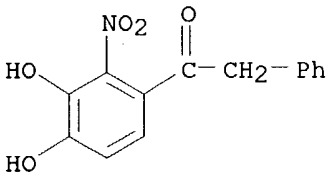
present case

AB Title compds. I [wherein R1 and R2 = independently H or (un)substituted alkanoyl, aroyl, alkoxycarbonyl, or alkylcarbamoyl; R3 = H or (un)substituted alkanoyl or aroyl; R4 = (un)substituted alkyl or aryl; or R4 taken together with R3 = (un)substituted carbocycle; A = O, NR5, or (un)substituted alkylidene; R5 = NHR6 or OR7; R6 = (un)substituted alkyl or aryl; R7 = H, alkyl, or alkanoyl; with provisos] were prepared as catechol O-Me transferase (COMT) inhibitors. In COMT oral

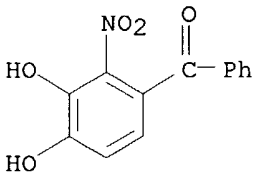
bioavailability, half-life, and brain access assays, some invention compds. demonstrated enhanced access to the brain and limited activity in the periphery offering improved selectivity for mood disorder therapy. Others demonstrated limited access to the brain and enhanced activity in the periphery offering improved selectivity for treatment of Parkinson's disease and parkinsonian disorders, gastrointestinal disturbances, edema formation states and hypertension. Thus, bromination of 3,4-dihydroxy-2-nitroacetophenone with phenyltrimethylammonium tribromide in THF to give the α-bromoketone, followed by addition of morpholine in MeCN, afforded 1-(3,4-dihydroxy-2-nitrophenyl)-2-morpholin-4-ylethanone. The latter inhibited COMT activity in homogenates of rat liver and brain and SK-N-SH cells at 0.8 0.2%, 13 0%, and 27 0%, resp., compared to control.

IT **383382-82-9P**, 1-(3,4-Dihydroxy-2-nitrophenyl)-2-phenylethanone
383382-84-1P, (3,4-Dihydroxy-2-nitrophenyl)phenylmethanone
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; preparation of substituted nitrated catechols as COMT inhibitors for treatment of central and peripheral nervous system disorders)

RN 383382-82-9 CAPLUS
CN Ethanone, 1-(3,4-dihydroxy-2-nitrophenyl)-2-phenyl- (9CI) (CA INDEX NAME)

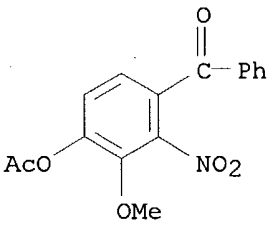


RN 383382-84-1 CAPLUS
CN Methanone, (3,4-dihydroxy-2-nitrophenyl)phenyl- (9CI) (CA INDEX NAME)

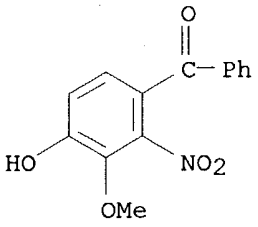


IT **383382-96-5P**, Acetic acid 4-benzoyl-2-methoxy-3-nitrophenyl ester
383382-98-7P, (4-Hydroxy-3-methoxy-2-nitrophenyl)phenylmethanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted nitrated catechols as COMT inhibitors for treatment of central and peripheral nervous system disorders)

RN 383382-96-5 CAPLUS
CN Methanone, [4-(acetyloxy)-3-methoxy-2-nitrophenyl]phenyl- (9CI) (CA INDEX NAME)

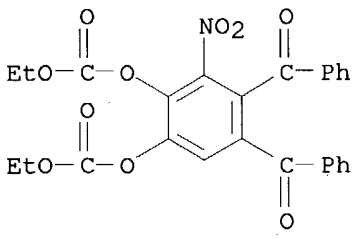


RN 383382-98-7 CAPLUS
CN Methanone, (4-hydroxy-3-methoxy-2-nitrophenyl)phenyl- (9CI) (CA INDEX NAME)

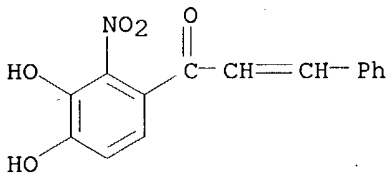


IT **383382-43-2P**, Carbonic acid 4,5-dibenzoyl-2-ethoxycarbonyloxy-3-nitrophenyl ester ethyl ester **383382-59-0P**, 1-(3,4-Dihydroxy-2-nitrophenyl)-3-phenylpropenone **383382-83-0P**, Butyric acid 3-benzoyl-6-butyryloxy-2-nitrophenyl ester **383382-85-2P**, Carbonic acid 4-benzoyl-2-ethoxycarbonyloxy-3-nitrophenyl ester ethyl ester **383382-86-3P**, Butyric acid 6-butyryloxy-2-nitro-3-(3-phenylpropionyl)phenyl ester **383382-87-4P**, Carbonic acid 2-ethoxycarbonyloxy-3-nitro-4-(3-phenylpropionyl)phenyl ester ethyl ester **383382-88-5P**, Acetic acid 6-acetoxy-2-nitro-3-(3-phenylacryloyl)phenyl ester **383382-89-6P**, Acetic acid 6-acetoxy-2-nitro-3-phenylacetylphenyl ester **383382-90-9P**, Butyric acid 6-butyryloxy-2-nitro-3-phenylacetylphenyl ester **383382-91-0P**, Carbonic acid 2-ethoxycarbonyloxy-3-nitro-4-phenylacetylphenyl ester ethyl ester **383382-92-1P**, Acetic acid 6-acetoxy-2-nitro-3-(4-phenylbutyryl)phenyl ester **383382-93-2P**, Acetic acid 6-butyryloxy-2-nitro-3-(4-phenylbutyryl)phenyl ester **383382-95-4P**, Carbonic acid 2-ethoxycarbonyloxy-3-nitro-4-(4-phenylbutyryl)phenyl ester ethyl ester **383382-99-8P**, 1-(3,4-Dihydroxy-2-nitrophenyl)-3-phenylpropan-1-one **383383-00-4P**, 1-(3,4-Dihydroxy-2-nitrophenyl)-4-phenylbutan-1-one **383383-03-7P**, Butyric acid 6-butyryloxy-2-nitro-3-(4-phenylbutyryl)phenyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted nitrated catechols as COMT inhibitors for treatment of central and peripheral nervous system disorders)

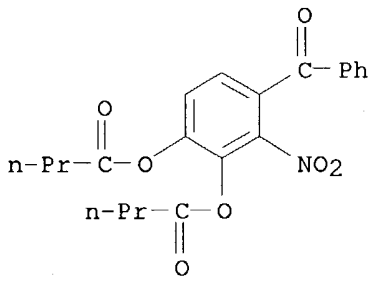
RN 383382-43-2 CAPLUS
CN Carbonic acid, 4,5-dibenzoyl-3-nitro-1,2-phenylene diethyl ester (9CI) (CA INDEX NAME)



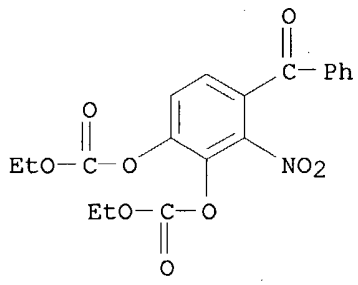
RN 383382-59-0 CAPLUS
CN 2-Propen-1-one, 1-(3,4-dihydroxy-2-nitrophenyl)-3-phenyl- (9CI) (CA INDEX NAME)



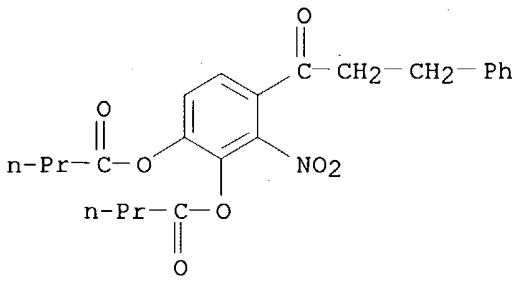
RN 383382-83-0 CAPLUS
CN Butanoic acid, 4-benzoyl-3-nitro-1,2-phenylene ester (9CI) (CA INDEX NAME)



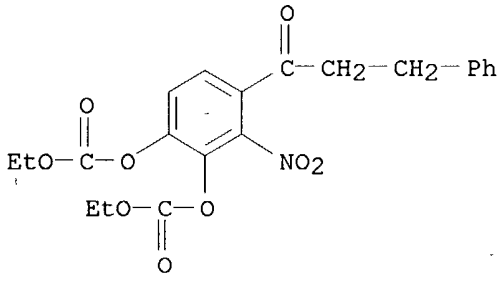
RN 383382-85-2 CAPLUS
CN Carbonic acid, 4-benzoyl-3-nitro-1,2-phenylene diethyl ester (9CI) (CA INDEX NAME)



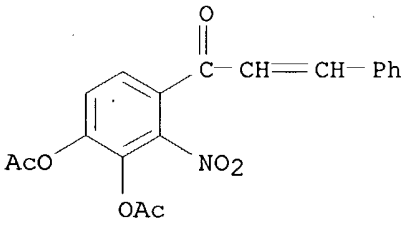
RN 383382-86-3 CAPLUS
CN Butanoic acid, 3-nitro-4-(1-oxo-3-phenylpropyl)-1,2-phenylene ester (9CI) (CA INDEX NAME)



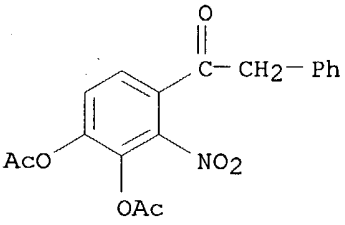
RN 383382-87-4 CAPLUS
CN Carbonic acid, 3-nitro-4-(1-oxo-3-phenylpropyl)-1,2-phenylene diethyl ester (9CI) (CA INDEX NAME)



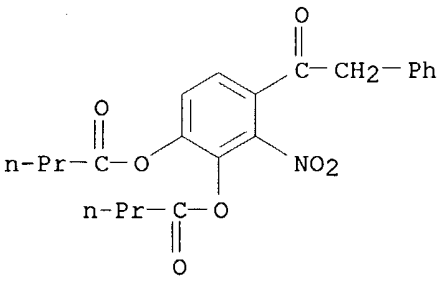
RN 383382-88-5 CAPLUS
CN 2-Propen-1-one, 1-[3,4-bis(acetyloxy)-2-nitrophenyl]-3-phenyl- (9CI) (CA INDEX NAME)



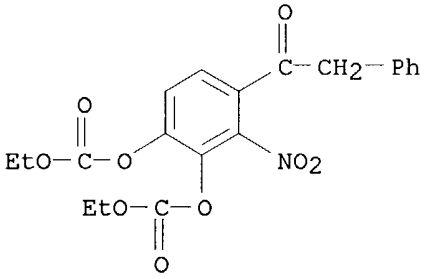
RN 383382-89-6 CAPLUS
CN Ethanone, 1-[3,4-bis(acetyloxy)-2-nitrophenyl]-2-phenyl- (9CI) (CA INDEX NAME)



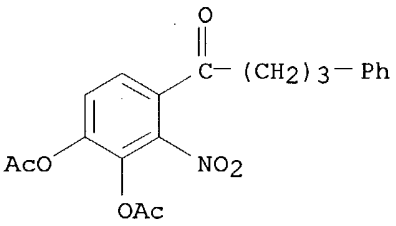
RN 383382-90-9 CAPLUS
CN Butanoic acid, 3-nitro-4-(phenylacetyl)-1,2-phenylene ester (9CI) (CA INDEX NAME)



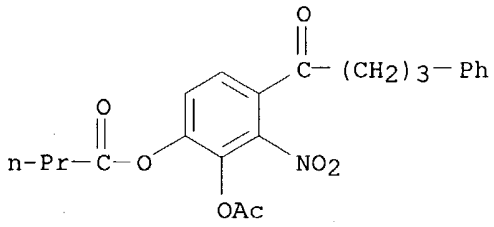
RN 383382-91-0 CAPLUS
CN Carbonic acid, 3-nitro-4-(phenylacetyl)-1,2-phenylene diethyl ester (9CI) (CA INDEX NAME)



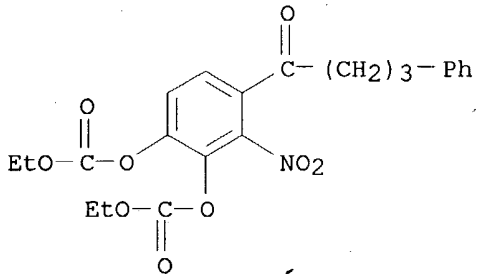
RN 383382-92-1 CAPLUS
CN 1-Butanone, 1-[3,4-bis(acetyloxy)-2-nitrophenyl]-4-phenyl- (9CI) (CA INDEX NAME)



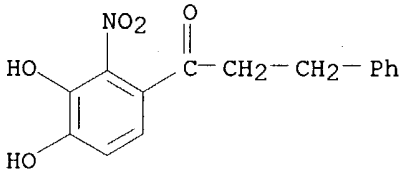
RN 383382-93-2 CAPLUS
CN Butanoic acid, 2-(acetyloxy)-3-nitro-4-(1-oxo-4-phenylbutyl)phenyl ester (9CI) (CA INDEX NAME)



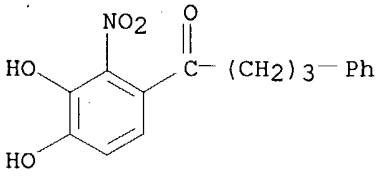
RN 383382-95-4 CAPLUS
CN Carbonic acid, 3-nitro-4-(1-oxo-4-phenylbutyl)-1,2-phenylene diethyl ester (9CI) (CA INDEX NAME)



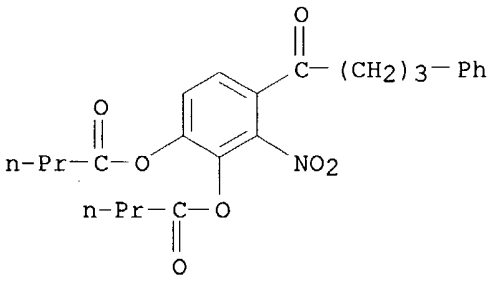
RN 383382-99-8 CAPLUS
CN 1-Propanone, 1-(3,4-dihydroxy-2-nitrophenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 383383-00-4 CAPLUS
CN 1-Butanone, 1-(3,4-dihydroxy-2-nitrophenyl)-4-phenyl- (9CI) (CA INDEX NAME)

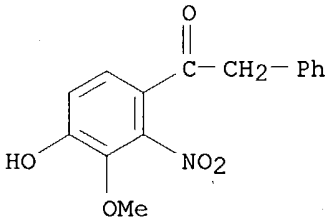


RN 383383-03-7 CAPLUS
CN Butanoic acid, 3-nitro-4-(1-oxo-4-phenylbutyl)-1,2-phenylene ester (9CI) (CA INDEX NAME)

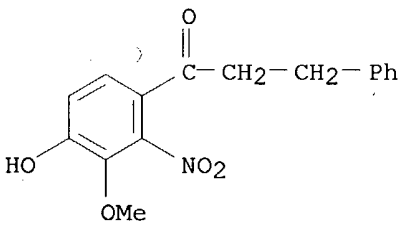


IT **383383-05-9**, 1-(4-Hydroxy-3-methoxy-2-nitrophenyl)-2-phenylethanone **383383-07-1**, 1-(4-Hydroxy-3-methoxy-2-nitrophenyl)-3-phenylpropan-1-one **383383-09-3**, 1-(4-Hydroxy-3-methoxy-2-nitrophenyl)-4-phenylbutan-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of substituted nitrated catechols as COMT inhibitors for treatment of central and peripheral nervous system disorders)

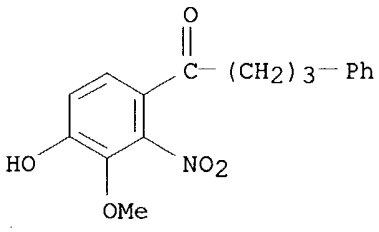
RN 383383-05-9 CAPLUS
CN Ethanone, 1-(4-hydroxy-3-methoxy-2-nitrophenyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 383383-07-1 CAPLUS
CN 1-Propanone, 1-(4-hydroxy-3-methoxy-2-nitrophenyl)-3-phenyl- (9CI) (CA INDEX NAME)

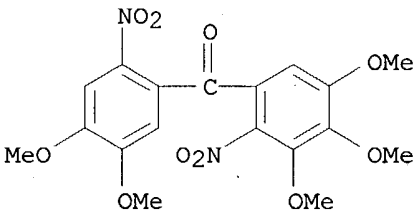


RN 383383-09-3 CAPLUS
CN 1-Butanone, 1-(4-hydroxy-3-methoxy-2-nitrophenyl)-4-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1971:518144 CAPLUS
DOCUMENT NUMBER: 75:118144
TITLE: Polycyclic compounds. II. Synthesis of 2,3,4,5,6-pentamethoxy- and 2,3,4,6,7-pentamethoxyfluorenones and structures of intermediate nitro compounds
AUTHOR(S): Pol, V. A.; Kulkarni, A. B.
CORPORATE SOURCE: Dep. Chem., Univ. Bombay, Bombay, India
SOURCE: Indian Journal of Chemistry (1971), 9(7), 615-18
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 3,4,5,3',4'-Pentamethoxy-2-nitrobenzophenone (I), obtained by controlled nitration of 3,4,3',4',5'-pentamethoxybenzophenone, on reduction followed by cyclization of the diazotized amino compound gives 2,3,4,5,6-pentamethoxy- and 2,3,4,6,7-pentamethoxyfluorenones. The structures of the intermediate, 4,5,3',4',5'-pentamethoxy-2,2'-dinitrobenzophenone, and 4,5,3',4',5 entaoxy-2-nitrobenzophenone are established unambiguously.
IT **33651-81-9P 33651-82-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33651-81-9 CAPLUS
CN Benzophenone, 3,4,4',5,5'-pentamethoxy-2,2'-dinitro- (8CI) (CA INDEX NAME)



RN 33651-82-0 CAPLUS
CN Benzophenone, 3,3',4,4',5-pentamethoxy-2-nitro- (8CI) (CA INDEX NAME)

aq/885,855